

Pressure dependence of electronic states in secondary explosives

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It is known that material porosity enhances shock sensitivity and it is assumed that localized heating initiates reactions at defect sites. However, a wealth of evidence indicates that the mechanism may not be thermal heating, but rather spontaneous pressure-induced decomposition. This alternate mechanism is postulated to involve shock-induced changes in the electronic structure of the material, in which instantaneous reactions occur at the shock front, assisted by local distortion of electronic structure at defect sites. At present, no definitive measurement or calculation has proven or disproven this mechanism. We will present electronic absorption measurements of explosive powders from up to 9 GPa and surface specific absorption measurements of thin-film explosives at ambient pressures using electronic sum frequency spectroscopy. Measurements will be compared with DFT models for the pressure dependence of electronic states to determine pressure-induced band-gap compression may contribute to the rate shock initiation.